Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Bromo-5-methoxy-*N*′-[(*E*)-(2-nitrophenyl)methylene]benzohydrazide

H. S. Yathirajan,[a] B. K. Sarojini,[b] B. Narayana,[c] K. Sunil[c] and Michael Bolte[d]*

[a]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, [b]Department of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, [c]Department of Studies in Chemistry, Mangalore University, Mangalagangotri 574 199, India, and [d]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany
Correspondence e-mail: bolte@chemie.uni-frankfurt.de

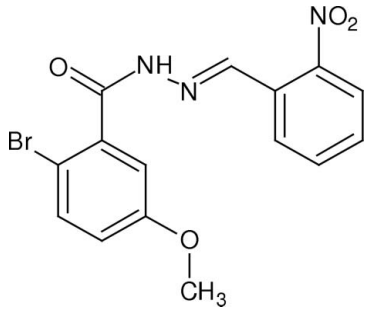
Received 19 April 2007; accepted 24 April 2007

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.091; data-to-parameter ratio = 16.4.

Geometric parameters of the title compound, $C_{15}H_{12}BrN_3O_4$, a Schiff base, are in the usual ranges. There are two molecules in the asymmetric unit, differing in the dihedral angles between the aromatic rings and the central CO—NH—N=C unit. Furthermore, the $C_{ar}—C_{ar}—O—CH_3$ torsion angles differ by almost 180°. The crystal packing is stabilized by N—H···O hydrogen bonds.

Related literature

For related structures, see: He *et al.* (2005), Zhen *et al.* (2005*a*,*b*), Diao *et al.* (2005). For related literature, see: El-Masry *et al.* (2000); Pandey *et al.* (1999); Singh *et al.* (1988); Hodnett *et al.* (1970); Desai *et al.* (2001); Aydoğan *et al.* (2001); Taggi *et al.* (2002).



Experimental

Crystal data

$C_{15}H_{12}BrN_3O_4$
M_r = 378.19
Triclinic, $P\overline{1}$
a = 8.1611 (6) Å
b = 9.0279 (6) Å
c = 21.3467 (15) Å
α = 85.585 (6)°
β = 89.441 (6)°
γ = 75.912 (5)°
V = 1520.88 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.73 mm^{-1}
T = 173 (2) K
0.36 × 0.33 × 0.32 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.401, T_{max} = 0.426
22860 measured reflections
7003 independent reflections
5849 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.091
S = 1.01
7003 reflections
426 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.99 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1A^{i}	0.86 (3)	2.09 (3)	2.863 (2)	149 (3)
N1A—H1A···O1	0.89 (3)	2.00 (3)	2.872 (3)	165 (3)

Symmetry code: (i) $x-1, y, z$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

KS thanks the Department of Studies in Chemistry, Mangalore University for research facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2279).

References

Aydoğan, F., Öcal, N., Turgut, Z. & Yolaçan, C. (2001). *Bull. Korean Chem. Soc.* **22**, 476–480.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Desai, S. B., Desai, P. B. & Desai, K. R. (2001). *Heterocycl. Commun.* **7**, 83–90.
Diao, C.-H., Yu, M., Chen, X., Jing, Z.-L. & Deng, Q.-L. (2005). *Acta Cryst.* E**61**, o3500–o3501.
El-Masry, A. H., Fahmy, H. H. & Abdelwahed, S. H. A. (2000). *Molecules*, **5**, 1429-1438.
He, Y.-Z. & Liu, D.-Z. (2005). *Acta Cryst.* E**61**, o3855–o3856.
Hodnett, E. M. & Dunn, W. J. (1970). *J. Med. Chem.* **13**, 768–770.
Pandey, S. N., Sriram, D., Nath, G. & De Clercq, E. (1999). *Il Farmaco*, **54**, 624–628.
Sheldrick, G. M. (1991). *SHELXTL-Plus*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Singh, W. M. & Dash, B. C. (1988). *Pesticides*, **22**, 33–37.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Taggi, A. E., Hafez, A. M., Wack, H., Young, B., Ferraris, D. & Lectka, T. (2002). *J. Am. Chem. Soc.* **124**, 6626–6635.
Zhen, X.-L. & Han, J.-R. (2005*a*). *Acta Cryst.* E**61**, o4282–o4284.
Zhen, X.-L. & Han, J.-R. (2005*b*). *Acta Cryst.* E**61**, o4360–o4361.

supplementary materials

Acta Cryst. (2007). E**63**, o2719 [**doi:10.1107/S1600536807020375**]

2-Bromo-5-methoxy-*N*'-[(*E*)-(2-nitrophenyl)methylene]benzohydrazide

H. S. Yathirajan, B. K. Sarojini, B. Narayana, K. Sunil and M. Bolte

Comment

Schiff bases are used as substrates in the preparation of number of industrial and biologically active compounds via ring closure, cycloaddition and replacement reactions. Moreover, Schiff bases are also known to have biological activities such as antimicrobial, antifungal, antitumor and as herbicides. Schiff bases have also been employed as ligands for complexation of metal ions. On the industrial scale, they have wide range of applications such as dyes and pigments. A new Schiff base, $C_{15}H_{12}BrN_3O_4$, was synthesized and its crystal structure is reported.

There are two molecules in the asymmetric unit differing in the dihedral angles between the aromatic rings and the central CO—NH—N=C unit [N2—C2—C21—C22 = 159.2 (2)°, N2A—C2A—C21A—C22A = -169.3 (2)°, O1—C1—C11—C12 = 74.2 (3)° and O1A—C1A—C11A—C12A = 104.5 (3)°]. The crystal packing is stabilized by N—H···O hydrogen bonds.

Experimental

A mixture of 2-bromo-5-methoxybenzohydrazide (1.22 g, 0.005 mol) and 2-nitrobenzaldehyde (0.75 g, 0.005 mol) in 25 ml of absolute ethanol containing 2 drops of 4 M sulfuric acid was refluxed for about 3 hours. On cooling, the solid separated was filtered and recrystallized from a mixture of (5:5) DMF & acetone (m.p.: 486-488 K). Analysis for $C_{15}H_{12}BrN_3O_4$: Found (Calculated): C : 47.56 (47.64); H:3.14 (3.20); N:11.04% (11.11%).

Refinement

All H atoms were found in a difference map, and the ones of the NH groups were refined freely. The rest H atoms were refined using a riding model with $C_{aromatic}$—H = 0.95 Å, C_{methyl}—H = 0.98Å or $C_{methylene}$—H = 0.99Å and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(C_{methyl}). The methyl group was allowed to rotate but not to tip.

Figures

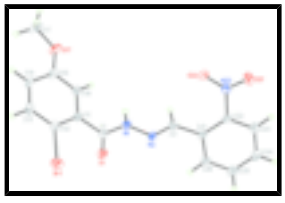


Fig. 1. Perspective view of molecule one in the asymmetric unit of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

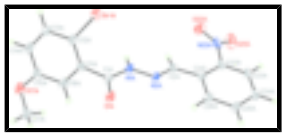


Fig. 2. Perspective view of molecule two in the asymmetric unit of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

2-Bromo-5-methoxy-*N*'-[(*E*)-(2-nitrophenyl)methylene]benzohydrazide

Crystal data

$C_{15}H_{12}BrN_3O_4$	$Z = 4$
$M_r = 378.19$	$F_{000} = 760$
Triclinic, $P\overline{1}$	$D_x = 1.652$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.1611$ (6) Å	Cell parameters from 21874 reflections
$b = 9.0279$ (6) Å	$\theta = 2.5$–26.8º
$c = 21.3467$ (15) Å	$\mu = 2.73$ mm^{-1}
$\alpha = 85.585$ (6)º	$T = 173$ (2) K
$\beta = 89.441$ (6)º	Block, colourless
$\gamma = 75.912$ (5)º	0.36 × 0.33 × 0.32 mm
$V = 1520.88$ (18) Å^3	

Data collection

Stoe IPDSII two-circle diffractometer	7003 independent reflections
Radiation source: fine-focus sealed tube	5849 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.061$
$T = 173$(2) K	$\theta_{max} = 27.6$º
ω scans	$\theta_{min} = 2.6$º
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	$h = -10 \rightarrow 10$
$T_{min} = 0.401$, $T_{max} = 0.426$	$k = -11 \rightarrow 11$
22860 measured reflections	$l = -27 \rightarrow 27$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 0.1348P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.091$	$\Delta\rho_{max} = 0.99$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.82$ e Å^{-3}
7003 reflections	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
426 parameters	Extinction coefficient: 0.0124 (9)
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.57284 (3)	0.71784 (3)	0.426996 (11)	0.02848 (8)
C1	0.5711 (3)	0.7471 (3)	0.27886 (10)	0.0187 (4)
O1	0.7255 (2)	0.7090 (2)	0.27580 (9)	0.0286 (4)
N1	0.4720 (2)	0.8821 (2)	0.25625 (9)	0.0196 (4)
H1	0.366 (4)	0.904 (3)	0.2649 (13)	0.019 (7)*
N2	0.5393 (2)	0.9885 (2)	0.22119 (8)	0.0183 (4)
C2	0.4284 (3)	1.1108 (3)	0.20414 (10)	0.0187 (4)
H2	0.3140	1.1220	0.2163	0.022*
C11	0.4685 (3)	0.6411 (2)	0.30862 (10)	0.0179 (4)
C12	0.4638 (3)	0.6110 (3)	0.37360 (10)	0.0202 (4)
C13	0.3702 (3)	0.5126 (3)	0.39970 (11)	0.0234 (5)
H13	0.3714	0.4899	0.4439	0.028*
C14	0.2756 (3)	0.4475 (3)	0.36165 (11)	0.0240 (5)
H14	0.2112	0.3807	0.3797	0.029*
C15	0.2745 (3)	0.4802 (3)	0.29653 (11)	0.0220 (4)
C16	0.3741 (3)	0.5756 (3)	0.27024 (10)	0.0208 (4)
H16	0.3768	0.5953	0.2259	0.025*
O17	0.1820 (2)	0.4259 (2)	0.25485 (9)	0.0311 (4)
C17	0.0475 (3)	0.3619 (3)	0.27988 (14)	0.0342 (6)
H17A	0.0946	0.2731	0.3093	0.051*
H17B	−0.0110	0.3297	0.2454	0.051*
H17C	−0.0326	0.4393	0.3020	0.051*
C21	0.4792 (3)	1.2352 (3)	0.16530 (10)	0.0181 (4)
C22	0.3661 (3)	1.3493 (3)	0.12820 (10)	0.0189 (4)
C23	0.4140 (3)	1.4700 (3)	0.09437 (11)	0.0249 (5)
H23	0.3337	1.5450	0.0696	0.030*
C24	0.5812 (3)	1.4787 (3)	0.09743 (12)	0.0287 (5)
H24	0.6163	1.5600	0.0747	0.034*
C25	0.6968 (3)	1.3684 (3)	0.13376 (12)	0.0273 (5)
H25	0.8108	1.3752	0.1362	0.033*
C26	0.6471 (3)	1.2473 (3)	0.16684 (10)	0.0221 (4)
H26	0.7286	1.1718	0.1909	0.027*
N22	0.1860 (2)	1.3483 (2)	0.12283 (9)	0.0221 (4)

O21	0.0829 (2)	1.4713 (2)	0.11166 (10)	0.0352 (4)
O22	0.1468 (2)	1.2248 (2)	0.12971 (9)	0.0296 (4)
Br1A	0.70200 (3)	1.19678 (3)	0.331535 (11)	0.03073 (9)
C1A	1.0416 (3)	0.9286 (3)	0.32993 (10)	0.0188 (4)
O1A	1.1748 (2)	0.9686 (2)	0.33047 (8)	0.0265 (4)
N1A	0.9787 (2)	0.8805 (2)	0.27891 (9)	0.0211 (4)
H1A	0.889 (4)	0.841 (4)	0.2821 (15)	0.031 (8)*
N2A	1.0619 (2)	0.8881 (2)	0.22218 (9)	0.0201 (4)
C2A	1.0003 (3)	0.8349 (3)	0.17647 (10)	0.0213 (4)
H2A	0.9044	0.7934	0.1822	0.026*
C11A	0.9363 (3)	0.9301 (3)	0.38867 (10)	0.0198 (4)
C12A	0.7888 (3)	1.0420 (3)	0.39665 (11)	0.0221 (4)
C13A	0.7040 (3)	1.0488 (3)	0.45422 (11)	0.0246 (5)
H13A	0.6031	1.1258	0.4592	0.030*
C14A	0.7670 (3)	0.9439 (3)	0.50341 (11)	0.0253 (5)
H14A	0.7100	0.9488	0.5425	0.030*
C15A	0.9152 (3)	0.8296 (3)	0.49627 (11)	0.0231 (5)
C16A	0.9999 (3)	0.8239 (3)	0.43911 (11)	0.0223 (4)
H16A	1.1014	0.7475	0.4344	0.027*
O17A	0.9665 (2)	0.7305 (2)	0.54816 (8)	0.0321 (4)
C17A	1.1194 (4)	0.6155 (3)	0.54411 (12)	0.0323 (6)
H17D	1.1087	0.5494	0.5108	0.048*
H17E	1.1422	0.5538	0.5843	0.048*
H17F	1.2128	0.6640	0.5344	0.048*
C21A	1.0826 (3)	0.8397 (2)	0.11419 (10)	0.0184 (4)
C22A	1.0152 (3)	0.8091 (3)	0.05801 (10)	0.0201 (4)
C23A	1.1006 (3)	0.8080 (3)	0.00099 (11)	0.0242 (5)
H23A	1.0523	0.7838	−0.0360	0.029*
C24A	1.2573 (3)	0.8428 (3)	−0.00072 (11)	0.0246 (5)
H24A	1.3161	0.8443	−0.0393	0.029*
C25A	1.3278 (3)	0.8752 (3)	0.05375 (11)	0.0236 (5)
H25A	1.4345	0.9001	0.0524	0.028*
C26A	1.2426 (3)	0.8714 (3)	0.11056 (11)	0.0220 (4)
H26A	1.2942	0.8907	0.1478	0.026*
N22A	0.8456 (3)	0.7797 (3)	0.05512 (9)	0.0289 (5)
O21A	0.8153 (3)	0.7032 (3)	0.01402 (10)	0.0466 (6)
O22A	0.7404 (2)	0.8375 (3)	0.09338 (10)	0.0445 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03308 (14)	0.03262 (15)	0.02237 (12)	−0.01171 (10)	−0.00104 (9)	−0.00635 (9)
C1	0.0179 (10)	0.0197 (10)	0.0196 (10)	−0.0073 (8)	0.0003 (8)	0.0010 (8)
O1	0.0158 (7)	0.0255 (9)	0.0434 (10)	−0.0054 (7)	0.0025 (7)	0.0055 (8)
N1	0.0148 (9)	0.0210 (9)	0.0232 (9)	−0.0067 (7)	0.0038 (7)	0.0039 (7)
N2	0.0199 (9)	0.0191 (9)	0.0177 (8)	−0.0094 (7)	0.0020 (7)	0.0011 (7)
C2	0.0166 (9)	0.0232 (11)	0.0173 (9)	−0.0079 (8)	0.0016 (7)	0.0011 (8)
C11	0.0153 (9)	0.0174 (10)	0.0209 (10)	−0.0045 (8)	0.0025 (8)	0.0005 (8)

C12	0.0210 (10)	0.0195 (10)	0.0196 (10)	−0.0040 (8)	0.0005 (8)	−0.0009 (8)
C13	0.0265 (11)	0.0223 (11)	0.0199 (10)	−0.0045 (9)	0.0065 (9)	0.0021 (8)
C14	0.0246 (11)	0.0206 (11)	0.0271 (11)	−0.0079 (9)	0.0071 (9)	0.0024 (9)
C15	0.0215 (10)	0.0207 (11)	0.0251 (11)	−0.0075 (9)	0.0040 (9)	−0.0032 (9)
C16	0.0216 (10)	0.0230 (11)	0.0185 (10)	−0.0072 (9)	0.0031 (8)	−0.0004 (8)
O17	0.0316 (9)	0.0406 (11)	0.0294 (9)	−0.0234 (8)	0.0076 (7)	−0.0092 (8)
C17	0.0309 (13)	0.0412 (15)	0.0393 (14)	−0.0245 (12)	0.0080 (11)	−0.0083 (12)
C21	0.0206 (10)	0.0192 (10)	0.0160 (9)	−0.0077 (8)	0.0018 (8)	−0.0016 (8)
C22	0.0182 (10)	0.0206 (10)	0.0196 (10)	−0.0085 (8)	0.0001 (8)	−0.0009 (8)
C23	0.0272 (12)	0.0213 (11)	0.0257 (11)	−0.0071 (9)	−0.0001 (9)	0.0047 (9)
C24	0.0324 (13)	0.0263 (12)	0.0306 (12)	−0.0151 (10)	0.0079 (10)	0.0025 (10)
C25	0.0217 (11)	0.0335 (13)	0.0303 (12)	−0.0138 (10)	0.0039 (9)	−0.0020 (10)
C26	0.0185 (10)	0.0279 (12)	0.0202 (10)	−0.0070 (9)	−0.0010 (8)	0.0009 (9)
N22	0.0209 (9)	0.0231 (10)	0.0227 (9)	−0.0079 (8)	−0.0030 (7)	0.0034 (8)
O21	0.0243 (9)	0.0255 (9)	0.0515 (12)	−0.0013 (7)	−0.0046 (8)	0.0094 (8)
O22	0.0270 (9)	0.0253 (9)	0.0392 (10)	−0.0138 (7)	−0.0099 (7)	0.0068 (7)
Br1A	0.02832 (14)	0.03399 (15)	0.02517 (13)	0.00198 (10)	−0.00220 (9)	−0.00360 (10)
C1A	0.0164 (10)	0.0203 (10)	0.0198 (10)	−0.0041 (8)	0.0041 (8)	−0.0039 (8)
O1A	0.0203 (8)	0.0398 (10)	0.0235 (8)	−0.0133 (7)	0.0064 (6)	−0.0096 (7)
N1A	0.0187 (9)	0.0293 (10)	0.0189 (9)	−0.0119 (8)	0.0058 (7)	−0.0044 (7)
N2A	0.0192 (9)	0.0233 (9)	0.0176 (8)	−0.0055 (7)	0.0051 (7)	−0.0011 (7)
C2A	0.0194 (10)	0.0274 (12)	0.0191 (10)	−0.0096 (9)	0.0018 (8)	−0.0015 (8)
C11A	0.0173 (10)	0.0254 (11)	0.0191 (10)	−0.0092 (9)	0.0037 (8)	−0.0053 (8)
C12A	0.0220 (10)	0.0244 (11)	0.0208 (10)	−0.0060 (9)	0.0022 (8)	−0.0057 (8)
C13A	0.0190 (10)	0.0321 (13)	0.0241 (11)	−0.0064 (9)	0.0045 (9)	−0.0107 (9)
C14A	0.0226 (11)	0.0344 (13)	0.0228 (11)	−0.0128 (10)	0.0089 (9)	−0.0090 (9)
C15A	0.0249 (11)	0.0268 (12)	0.0207 (10)	−0.0119 (10)	0.0046 (9)	−0.0029 (9)
C16A	0.0191 (10)	0.0268 (11)	0.0223 (10)	−0.0072 (9)	0.0052 (8)	−0.0047 (9)
O17A	0.0354 (10)	0.0353 (10)	0.0232 (8)	−0.0057 (8)	0.0089 (7)	0.0029 (7)
C17A	0.0368 (14)	0.0314 (14)	0.0260 (12)	−0.0042 (11)	0.0022 (10)	0.0011 (10)
C21A	0.0198 (10)	0.0178 (10)	0.0173 (9)	−0.0046 (8)	−0.0002 (8)	0.0001 (8)
C22A	0.0199 (10)	0.0213 (11)	0.0200 (10)	−0.0075 (8)	−0.0010 (8)	0.0013 (8)
C23A	0.0288 (12)	0.0280 (12)	0.0168 (10)	−0.0092 (10)	−0.0001 (8)	−0.0009 (9)
C24A	0.0276 (12)	0.0262 (12)	0.0204 (10)	−0.0081 (9)	0.0046 (9)	0.0004 (9)
C25A	0.0214 (11)	0.0260 (12)	0.0253 (11)	−0.0099 (9)	0.0040 (9)	−0.0013 (9)
C26A	0.0223 (11)	0.0259 (12)	0.0202 (10)	−0.0095 (9)	−0.0001 (8)	−0.0033 (9)
N22A	0.0287 (11)	0.0424 (13)	0.0191 (9)	−0.0174 (10)	−0.0052 (8)	0.0057 (9)
O21A	0.0521 (13)	0.0743 (16)	0.0291 (10)	−0.0441 (12)	−0.0038 (9)	−0.0078 (10)
O22A	0.0220 (9)	0.0772 (17)	0.0362 (10)	−0.0146 (10)	0.0027 (8)	−0.0087 (10)

Geometric parameters (Å, °)

Br1—C12	1.905 (2)	Br1A—C12A	1.904 (2)
C1—O1	1.225 (3)	C1A—O1A	1.226 (3)
C1—N1	1.345 (3)	C1A—N1A	1.353 (3)
C1—C11	1.519 (3)	C1A—C11A	1.513 (3)
N1—N2	1.387 (2)	N1A—N2A	1.388 (2)
N1—H1	0.86 (3)	N1A—H1A	0.89 (3)
N2—C2	1.276 (3)	N2A—C2A	1.279 (3)

C2—C21	1.482 (3)	C2A—C21A	1.486 (3)
C2—H2	0.9500	C2A—H2A	0.9500
C11—C16	1.387 (3)	C11A—C12A	1.389 (3)
C11—C12	1.395 (3)	C11A—C16A	1.399 (3)
C12—C13	1.389 (3)	C12A—C13A	1.403 (3)
C13—C14	1.381 (4)	C13A—C14A	1.373 (4)
C13—H13	0.9500	C13A—H13A	0.9500
C14—C15	1.398 (3)	C14A—C15A	1.401 (4)
C14—H14	0.9500	C14A—H14A	0.9500
C15—O17	1.365 (3)	C15A—O17A	1.370 (3)
C15—C16	1.405 (3)	C15A—C16A	1.395 (3)
C16—H16	0.9500	C16A—H16A	0.9500
O17—C17	1.440 (3)	O17A—C17A	1.423 (3)
C17—H17A	0.9800	C17A—H17D	0.9800
C17—H17B	0.9800	C17A—H17E	0.9800
C17—H17C	0.9800	C17A—H17F	0.9800
C21—C26	1.402 (3)	C21A—C22A	1.398 (3)
C21—C22	1.402 (3)	C21A—C26A	1.403 (3)
C22—C23	1.394 (3)	C22A—C23A	1.396 (3)
C22—N22	1.478 (3)	C22A—N22A	1.474 (3)
C23—C24	1.388 (3)	C23A—C24A	1.389 (3)
C23—H23	0.9500	C23A—H23A	0.9500
C24—C25	1.386 (4)	C24A—C25A	1.384 (3)
C24—H24	0.9500	C24A—H24A	0.9500
C25—C26	1.396 (3)	C25A—C26A	1.395 (3)
C25—H25	0.9500	C25A—H25A	0.9500
C26—H26	0.9500	C26A—H26A	0.9500
N22—O21	1.228 (3)	N22A—O21A	1.220 (3)
N22—O22	1.230 (3)	N22A—O22A	1.229 (3)
O1—C1—N1	125.8 (2)	O1A—C1A—N1A	124.10 (19)
O1—C1—C11	122.3 (2)	O1A—C1A—C11A	120.4 (2)
N1—C1—C11	111.86 (18)	N1A—C1A—C11A	115.47 (19)
C1—N1—N2	120.90 (18)	C1A—N1A—N2A	118.40 (18)
C1—N1—H1	119.3 (18)	C1A—N1A—H1A	121 (2)
N2—N1—H1	119.8 (18)	N2A—N1A—H1A	121 (2)
C2—N2—N1	112.79 (18)	C2A—N2A—N1A	115.31 (19)
N2—C2—C21	119.58 (19)	N2A—C2A—C21A	118.3 (2)
N2—C2—H2	120.2	N2A—C2A—H2A	120.8
C21—C2—H2	120.2	C21A—C2A—H2A	120.8
C16—C11—C12	119.29 (19)	C12A—C11A—C16A	119.0 (2)
C16—C11—C1	119.10 (19)	C12A—C11A—C1A	122.5 (2)
C12—C11—C1	121.6 (2)	C16A—C11A—C1A	118.2 (2)
C13—C12—C11	120.6 (2)	C11A—C12A—C13A	120.8 (2)
C13—C12—Br1	119.77 (17)	C11A—C12A—Br1A	121.18 (16)
C11—C12—Br1	119.51 (16)	C13A—C12A—Br1A	117.95 (18)
C14—C13—C12	120.3 (2)	C14A—C13A—C12A	119.8 (2)
C14—C13—H13	119.8	C14A—C13A—H13A	120.1
C12—C13—H13	119.8	C12A—C13A—H13A	120.1
C13—C14—C15	119.9 (2)	C13A—C14A—C15A	120.3 (2)

C13—C14—H14	120.0	C13A—C14A—H14A	119.8
C15—C14—H14	120.0	C15A—C14A—H14A	119.8
O17—C15—C14	124.8 (2)	O17A—C15A—C16A	124.8 (2)
O17—C15—C16	115.7 (2)	O17A—C15A—C14A	115.5 (2)
C14—C15—C16	119.5 (2)	C16A—C15A—C14A	119.7 (2)
C11—C16—C15	120.4 (2)	C15A—C16A—C11A	120.4 (2)
C11—C16—H16	119.8	C15A—C16A—H16A	119.8
C15—C16—H16	119.8	C11A—C16A—H16A	119.8
C15—O17—C17	117.21 (19)	C15A—O17A—C17A	117.79 (18)
O17—C17—H17A	109.5	O17A—C17A—H17D	109.5
O17—C17—H17B	109.5	O17A—C17A—H17E	109.5
H17A—C17—H17B	109.5	H17D—C17A—H17E	109.5
O17—C17—H17C	109.5	O17A—C17A—H17F	109.5
H17A—C17—H17C	109.5	H17D—C17A—H17F	109.5
H17B—C17—H17C	109.5	H17E—C17A—H17F	109.5
C26—C21—C22	116.39 (19)	C22A—C21A—C26A	116.33 (19)
C26—C21—C2	119.9 (2)	C22A—C21A—C2A	124.8 (2)
C22—C21—C2	123.7 (2)	C26A—C21A—C2A	118.8 (2)
C23—C22—C21	123.1 (2)	C23A—C22A—C21A	122.8 (2)
C23—C22—N22	115.7 (2)	C23A—C22A—N22A	115.6 (2)
C21—C22—N22	121.25 (18)	C21A—C22A—N22A	121.60 (19)
C24—C23—C22	118.8 (2)	C24A—C23A—C22A	118.9 (2)
C24—C23—H23	120.6	C24A—C23A—H23A	120.5
C22—C23—H23	120.6	C22A—C23A—H23A	120.5
C25—C24—C23	119.9 (2)	C25A—C24A—C23A	120.1 (2)
C25—C24—H24	120.1	C25A—C24A—H24A	120.0
C23—C24—H24	120.1	C23A—C24A—H24A	120.0
C24—C25—C26	120.6 (2)	C24A—C25A—C26A	120.1 (2)
C24—C25—H25	119.7	C24A—C25A—H25A	120.0
C26—C25—H25	119.7	C26A—C25A—H25A	120.0
C25—C26—C21	121.2 (2)	C25A—C26A—C21A	121.7 (2)
C25—C26—H26	119.4	C25A—C26A—H26A	119.1
C21—C26—H26	119.4	C21A—C26A—H26A	119.1
O21—N22—O22	123.3 (2)	O21A—N22A—O22A	123.4 (2)
O21—N22—C22	118.03 (19)	O21A—N22A—C22A	118.6 (2)
O22—N22—C22	118.63 (19)	O22A—N22A—C22A	117.9 (2)
O1—C1—N1—N2	5.9 (4)	O1A—C1A—N1A—N2A	−5.4 (3)
C11—C1—N1—N2	−172.86 (19)	C11A—C1A—N1A—N2A	174.89 (19)
C1—N1—N2—C2	−179.1 (2)	C1A—N1A—N2A—C2A	177.2 (2)
N1—N2—C2—C21	−178.92 (19)	N1A—N2A—C2A—C21A	179.8 (2)
O1—C1—C11—C16	−107.3 (3)	O1A—C1A—C11A—C12A	104.5 (3)
N1—C1—C11—C16	71.5 (3)	N1A—C1A—C11A—C12A	−75.8 (3)
O1—C1—C11—C12	74.2 (3)	O1A—C1A—C11A—C16A	−68.7 (3)
N1—C1—C11—C12	−106.9 (2)	N1A—C1A—C11A—C16A	111.0 (2)
C16—C11—C12—C13	2.1 (3)	C16A—C11A—C12A—C13A	−0.2 (3)
C1—C11—C12—C13	−179.4 (2)	C1A—C11A—C12A—C13A	−173.3 (2)
C16—C11—C12—Br1	−173.15 (17)	C16A—C11A—C12A—Br1A	176.51 (17)
C1—C11—C12—Br1	5.3 (3)	C1A—C11A—C12A—Br1A	3.4 (3)
C11—C12—C13—C14	−2.4 (4)	C11A—C12A—C13A—C14A	0.0 (4)

Br1—C12—C13—C14	172.88 (18)	Br1A—C12A—C13A—C14A	−176.78 (19)
C12—C13—C14—C15	0.3 (4)	C12A—C13A—C14A—C15A	−0.3 (4)
C13—C14—C15—O17	−178.0 (2)	C13A—C14A—C15A—O17A	−179.7 (2)
C13—C14—C15—C16	1.9 (4)	C13A—C14A—C15A—C16A	0.8 (4)
C12—C11—C16—C15	0.1 (3)	O17A—C15A—C16A—C11A	179.5 (2)
C1—C11—C16—C15	−178.3 (2)	C14A—C15A—C16A—C11A	−1.0 (4)
O17—C15—C16—C11	177.8 (2)	C12A—C11A—C16A—C15A	0.7 (3)
C14—C15—C16—C11	−2.1 (3)	C1A—C11A—C16A—C15A	174.1 (2)
C14—C15—O17—C17	15.5 (4)	C16A—C15A—O17A—C17A	1.6 (4)
C16—C15—O17—C17	−164.4 (2)	C14A—C15A—O17A—C17A	−177.9 (2)
N2—C2—C21—C26	−24.0 (3)	N2A—C2A—C21A—C22A	−169.3 (2)
N2—C2—C21—C22	159.2 (2)	N2A—C2A—C21A—C26A	13.2 (3)
C26—C21—C22—C23	−0.2 (3)	C26A—C21A—C22A—C23A	0.6 (3)
C2—C21—C22—C23	176.7 (2)	C2A—C21A—C22A—C23A	−176.9 (2)
C26—C21—C22—N22	179.8 (2)	C26A—C21A—C22A—N22A	−177.7 (2)
C2—C21—C22—N22	−3.2 (3)	C2A—C21A—C22A—N22A	4.7 (4)
C21—C22—C23—C24	−0.2 (4)	C21A—C22A—C23A—C24A	−1.8 (4)
N22—C22—C23—C24	179.7 (2)	N22A—C22A—C23A—C24A	176.6 (2)
C22—C23—C24—C25	−0.1 (4)	C22A—C23A—C24A—C25A	1.1 (4)
C23—C24—C25—C26	0.7 (4)	C23A—C24A—C25A—C26A	0.7 (4)
C24—C25—C26—C21	−1.2 (4)	C24A—C25A—C26A—C21A	−1.9 (4)
C22—C21—C26—C25	0.9 (3)	C22A—C21A—C26A—C25A	1.3 (3)
C2—C21—C26—C25	−176.1 (2)	C2A—C21A—C26A—C25A	179.0 (2)
C23—C22—N22—O21	−27.5 (3)	C23A—C22A—N22A—O21A	27.1 (3)
C21—C22—N22—O21	152.4 (2)	C21A—C22A—N22A—O21A	−154.4 (2)
C23—C22—N22—O22	152.5 (2)	C23A—C22A—N22A—O22A	−150.8 (2)
C21—C22—N22—O22	−27.6 (3)	C21A—C22A—N22A—O22A	27.7 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1A^{i}	0.86 (3)	2.09 (3)	2.863 (2)	149 (3)
N1A—H1A···O1	0.89 (3)	2.00 (3)	2.872 (3)	165 (3)

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

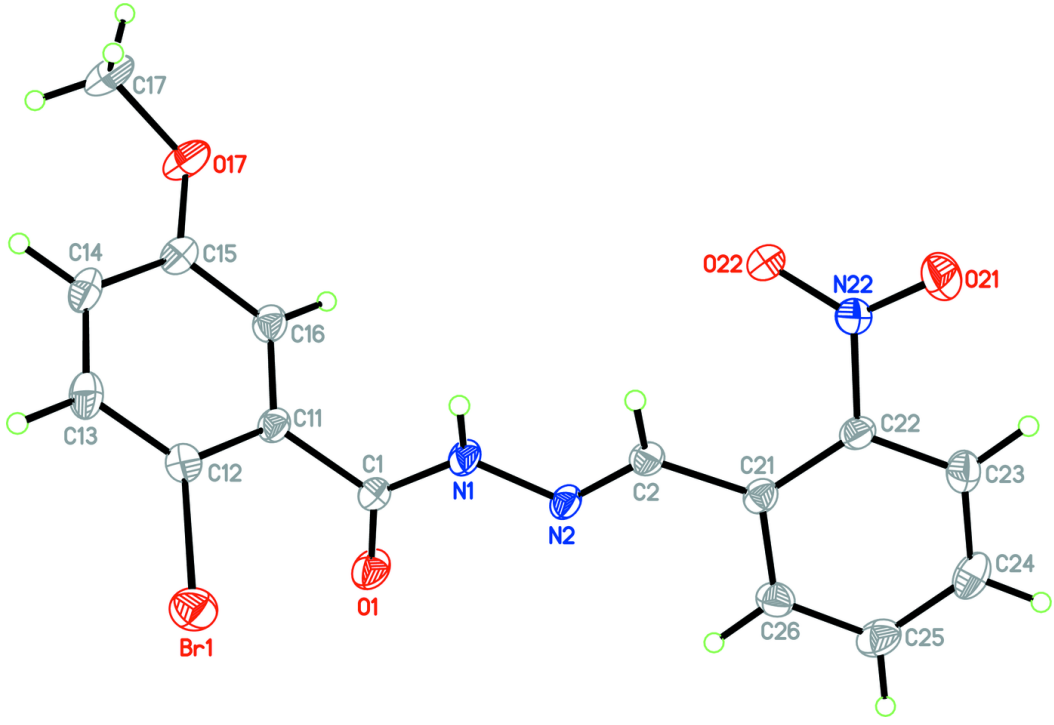
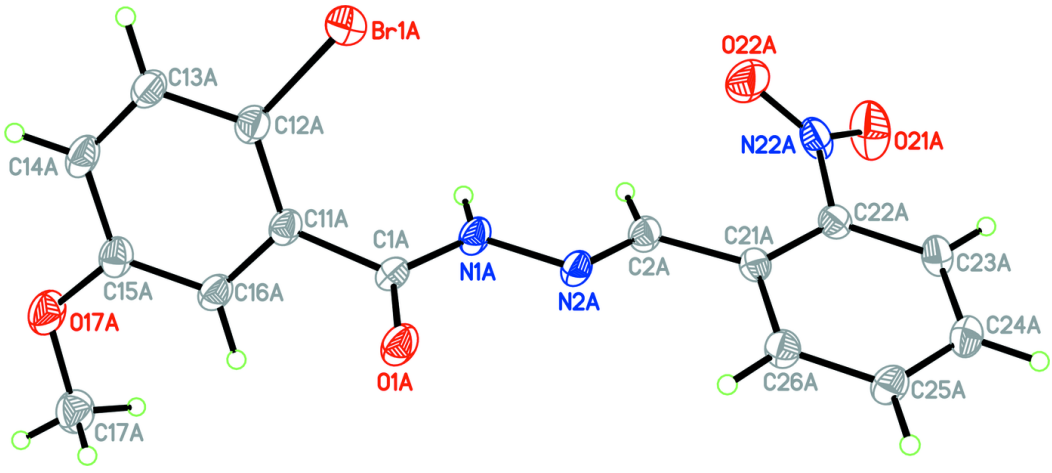

C17
O17
C14
C15
C16
C13
C11
C12
C1
N1
N2
C2
C21
C22
C23
C24
C25
C26
O22
N22
O21
O1
Br1

Fig. 2


Br1A
C13A
C12A
C14A
C11A
C1A
N1A
N2A
C2A
C21A
C22A
O22A
N22A
O21A
C23A
C24A
C15A
C16A
O17A
O1A
C26A
C25A
C17A